Revue des Energies Renouvelables Vol. 12 N°1 (2009) 55 – 62
DOI: https://doi.org/10.54966/jreen.v12i1.118

Numerical investigation of soot formation in diesel jet flame with KIVA-3V

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(reçu le 15 Février 2009 – accepté le 28 Mars 2009)

Abstract - *Diesel engines emit a Large amount of pollutants essentially soot particles. This paper describes a 3D modeling on platform of a 3-D code for engine thermodynamic simulation Kiva-3V. A Hiroyasu model for soot formation was used originally, it's a two-step Empirical model has been implanted in the code. This study was conducted to predict the emission of pollutants such soot more accurately and to enhance understanding of the pollutant formation process. The simulation was carried out by using a supercharged direct injected single cylinder diesel engine for heavy-duty applications.*

Résumé - *Les moteurs diesel émettent essentiellement un taux élevé d'espèces polluantes, en particulier la suie ou bien les particules solides. Ce papier décrit une modélisation en 3D utilisant un code de calcul numérique pour la simulation des moteurs Kiva-3V. Un modèle Hiroyasu pour la formation de la suie a été utilisé originalement. Ce modèle est validé en deus étapes empiriques de modélisation. Il a été implanté dans le code. Cette étude a été menée pour prédire plus correctement l'émission des polluants, tels que la suie et aussi pour comprendre et faciliter le processus de la formation des polluants. La simulation a été examinée sur un moteur diesel à un seul cylindre, à injection directe et pour les applications lourdes.*

Key words: Soot model - Flame - Simulation - Soot formation rate - Soot oxidation rate.

1. INTRODUCTION

Modeling the soot formation process remains a key topic in studies of diesel engine combustion. In order to minimize the formation process, in order to explore advanced engine operation modes and, in turn, to guide modern engine design and development, it is important that authentic soot models be used in multi-dimensional diesel simulations for providing reliable predictions of soot formation.

A Soot prediction in realistic systems is one of the most challenging problems in theoretical and applied combustion. Soot formation as a chemical process is very complicated and not fully understood up to the moment. Soot is one of the major pollutants produced by diesel engines.

Soot formation and modeling is one of the least investigated and understood combustion areas also Soot modeling has become increasingly important as legislation allows less and less soot to be emitted from diesel engines. Engine manufacturers need to find ways to reduce the amount of soot produced by their engines.

Computational Fluid Dynamics or CFD modeling in conjunction with proper soot models is a way of looking into the problem and finding ways to reduce the soot emissions.

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This is due to the complexity of the process, or the uncertainty in the chemical pathway, and the uncertainty about the coupling of these processes with fluid dynamics, heat transfer and turbulence [10].

A mechanism of soot formation and oxidation is very complex. We wanted to create a relatively simple model for direct use in a 3-dimensional diesel engine simulation.

Kiva3 [5] was used as a basic solver for thermodynamic and aerodynamic modeling [2], to which the soot model was implemented. The two-stage model of soot formation and oxidation based on Hiroyasu assumptions because the soot formation is highly influenced by a local state (e.g. local temperature, concentration of fuel etc.).

2. DESCRIPTION OF THE MODEL OF PREDICTION OF SOOT

Two-step empirical soot model

In the invited lecture at the first COMODIA conference in Tokyo in 1985, H. Hiroyasu reviewed the soot model that had been published between 1962 and 1984 [2]. Among those, the two steps empirical soot model of Hiroyasu is the most well known. A Hiroyasu model for soot formation was used at the simulation. Then this model was implemented into Kiva3 code and tried in 3-dimensional case.

In their two step model, Hiroyasu *et al.* (4) considered the soot formation process as involving only two reactions steps: 1- the formation step, in which soot is linked directly to fuel vapor molecules, and 2- the oxidation step, which describes the destruction of soot particles via the attack of molecular oxygen.

The net rate of change in soot mass is the difference between the rates of formation and oxidation {Eq. (1)}, [1].

Where the soot formation and oxidation rates are expressed in Arrhenius form {Eq. (1), Eq. (3)}, [1].

Soot formation rate is proportional to the mass of fuel vapor multiplied by an Arrhenius rate constant in the Hiroyasu's model.

$$\frac{dm_{soot}}{dt} = \left.\frac{dm_{soot}}{dt}\right|_{form} - \left.\frac{dm_{soot}}{dt}\right|_{oxid} \tag{1}$$

$$\frac{dm_{soot\_form}}{dt} = A_1 . \exp\left(-\frac{T_{A1}}{T}\right) . mfuelv . \left(\frac{p_{gas}}{p_{gas\_ref}}\right)^{n1} \tag{2}$$

$$\frac{dm_{soot\_oxid}}{dt} = A_2 . \exp\left(-\frac{T_{A2}}{T}\right) . (m_{soot})^{n2} . \left(\frac{p_{O_2}}{p_{O_2-ref}}\right)^{n3} \tag{3}$$

where [1]:

A_1 : Constant for soot formation [usually about 10^{-4} s^{-1}]

A_2 : Constant for soot oxidation [just used 4000 s^{-1} at n2 = 1]

T_{A1} : Activation temperature [6313 K]

T_{A2} : Activation temperature [7070 K]

m_{fuelv} : Currently vapor fuel mass [g]

p_{gas} : Pressure of gas [MPa]

$p_{gas-ref}$: Reference pressure of gas [0.1 MPa]

p_{O_2} : Partial pressure of O_2 [MPa]

p_{O_2-ref} : Reference partial pressure of O_2 [0.021 MPa]

$n1 = 1.8,\ n2 = 1.0,\ n3 = 1.0$

3. SIMULATED ENGINE

The calculation was done with a block-structured mesh. Since the simulated Engine is a direct injected diesel one with 1-hole injector, also the investigated engine is a 2-stroke supercharged direct injected single cylinder diesel engine for heavy-duty applications.

The simulations were usually run at 3100 rpm, start of injection 2 deg before TDC. Further engine data can be seen in the **Table 1**.

Table 1: Diesel engine specification

Bore (mm)	100
Stroke (mm)	95.5
Squish (mm)	9.55
Conrod length (mm)	169.2
Compression ratio	15 :1
Speed (rpm)	3100

and the parameters of simulation are presented in the **Table 2**. [3]

Table 2: Numerical conditions

Parameter	Value
Hole diameter (mm)	0.124
Hole length (mm)	1.2
Number of Hole	1
Injection timing (deg. BTDC)	2
Inlet air temperature (K)	530
Inlet air pressure (MPa)	60
Mass of fuel injected (g)	0.05
Fuel	Gasoline

4. MESH

The proposed mesh consists to the piston bowl. The calculation was done with a block-Structured mesh. The combustion chamber employs a bowl shape shows in Figure 1 [7].

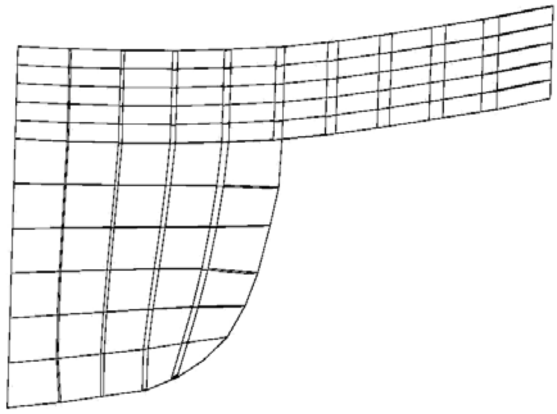


Fig. 1: Mesh of the simulated engine at TDC

5. RESULTS AND DISCUSSION

Results presented in the present section are obtained by using a supercharged direct injected single cylinder diesel engine for heavy-duty applications regard operating conditions at 3100 rpm, (Fig. 2).

Shows the history of modelled pressure variation inside the engine cylinder [9]. The pressure values simulated are higher near the end of injection. Its value max is 800 Mpa obtained by compression of 0.05 g of C_8H_{17}, at 2 BTDC initiate droplet injection and 12 crank angle degrees, the duration of injection pulse.

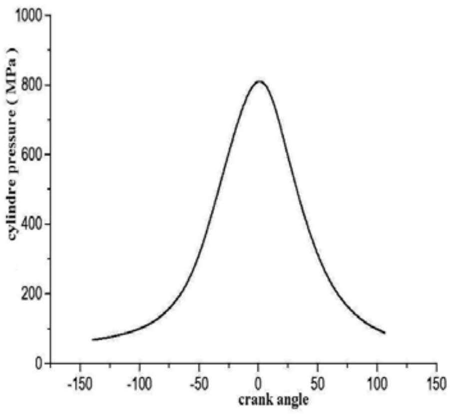


Fig. 2: In cylinder pressure

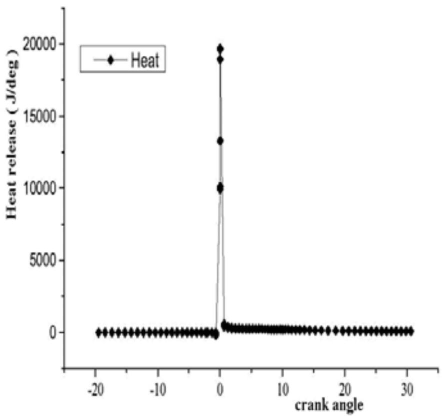


Fig. 3: Heat release

Therefore, both the magnitude and timing of occurrence of the peak pressure are precisely predicted by the model. The observed cylinder pressure profiles reflect the effects of in-cylinder heat release, heat transfer to the cylinder surfaces and work transfers [8]. At high engine speed, 3100 rpm, the heat release appears clearly distinguishable into a premixed phase and a diffusive phase.

Figure 3 shown apparent heat release rates computed from predicted pressure traces. Also shown is the fuel injection profile. Note that the heat release rate decreases from the start of injection to the start of combustion (ignition delay period) because of the fuel evaporation occurring during this period.

Figure 2, exhibits the peak shape that characterizes the direct injection diesel combustion. This peak due to premixed combustion strongly depends on the amount of Fuel that is prepared for combustion during the ignition delay period. As can be seen in Figure 3, the shape, timing, and magnitude of heat release peak predicted by the model. And spray dynamics, fuel droplet evaporation, fuel-air mixing, ignition delay, and combustion sub-models are properly working.

Figure 4 shows the density (g/cm^3) of Fuel (C_8H_{17}) inside the cylinder. It is predicted whit formation of soot. Note that higher temperature at 1300 K and plus. Its value max is 6.0×10^{-4} g/cm^3. This value obtained at end of injection, this is validating because the end of injection it's.

At presque 10 ATDC. This value increase successively.

Soot emission analysis

A Hiroyasu model for soot formation was used at the simulation. Then this model was implemented into KIVA 3 code and tried in 3-dimensional case [1]. Too high sensitivity to a residual fuel fraction during late expansion phase occurred giving overshoot soot formation without adequate oxidation.

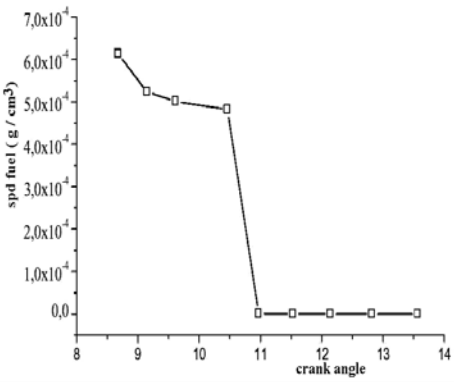


Fig. 4: Fuel density

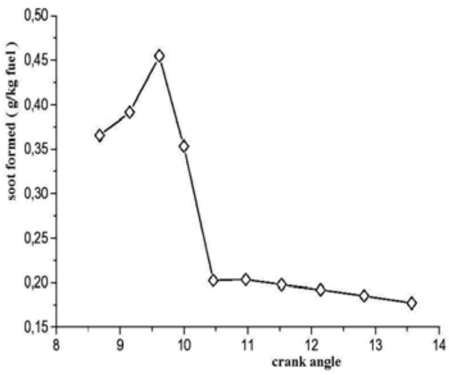
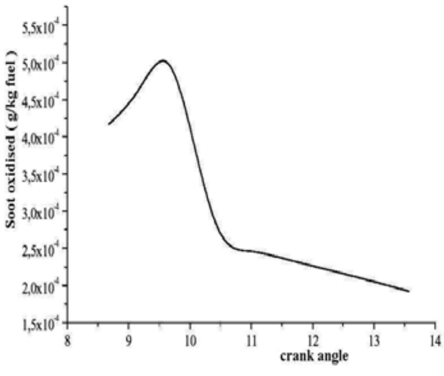


Fig. 5: Soot formed (g/kgfuel)

Soot processes in a turbulent diffusion flame have been studied numerically. Different modeling conditions have been considered. Soot results are presented in terms of soot mass in 1 kg of gasoline, net soot mass, rate of Formation and oxidation. Soot emission diagrams are reported in figures 5, 6 and 7.

In the diagrams of the figures 5, 6 and 7 could be distinguished three different zones: a first linear region; a zone of transition between the end of the linear region and the maximum of the plot; and the third part from the maximum to the end. It is interesting to notice that the linear portion of the plots depends almost exclusively on the concentration of vapor fuel and, therefore, for engine speeds.



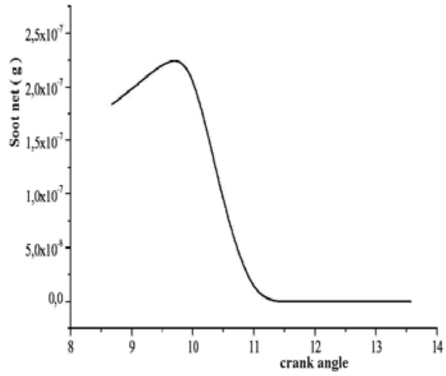


Fig. 6: Soot oxidised (g/kgfuel) Fig. 7: Soot net in cylinder

According to the used model, the temporal rate of soot production is given as the difference between the soot rate of formation and of oxidation {Eq. (1)}, thus, the Second part of the soot prediction plots represents the transition from the phase in which soot formation processes dominate to that in which the particles oxidation prevails. In fact, diagrams in figure 5, 6 and 7 show that soot oxidation follows the heat release curve of figure 3.

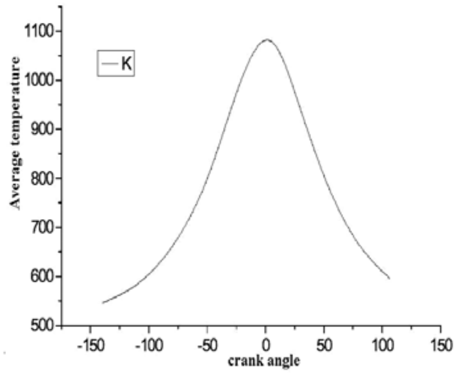


Fig. 8: Average temperature

Figure 8 shows the average temperature in the cylinder.

A section of a combustion chamber was created to visualize the computed results - figure 9 through figure 12. The axis of a cylinder is on the left hand side of figures, Figure 9 shown contour plots for temperature, at 3100 rpm and 10 crank angle degrees ATDC.

And figure 10 and figure 11 show mass fractions of fuel, oxygen. A vaporization of fuel causes the decrease in temperature (see temperature near to a cylinder axis). The premixed fuel/air Mixture near to the root of the spray begins to burn already at TDC (see increase of temperature). The burning is reflected by the local oxygen mass fraction decrease. The first traces of soot appear due to lack of oxygen and fuel cracking.

Figures 12 show KIVA graphic outputs at 10° crank angle degrees ATDC and at 3100 rpm. Such conditions were chosen in correspondence of the point in which the courses of the soot curves of figure.7 begin to separate. Corresponds to 10 deg after the TDC. Some originally big drops of fuel still exist, but the vaporized fuel mixed with air burns already and soot mass arises especially in the root of a spray [1]. Nearly all fuel has been burned till 90 deg after TDC, The soot mass continues oxidization slowly.

Figure 11 shows soot mass fractions in a combustion chamber cross-section. The pictures on the left hand side correspond to the soot Formation *Hiroyasu model*; the next two pictures correspond to 10 deg after TDC. Part of injected fuel is vaporised and combusted. The first traces of soot oxidised appeared and we can computed the soot net mass. The fuel burns with local lack of oxygen, therefore the soot concentration arises.

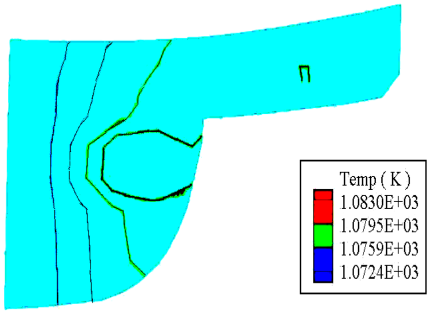


Fig. 9: Temperature contour

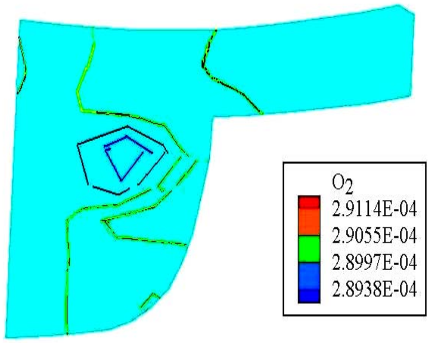


Fig. 10: Oxygen mass fraction

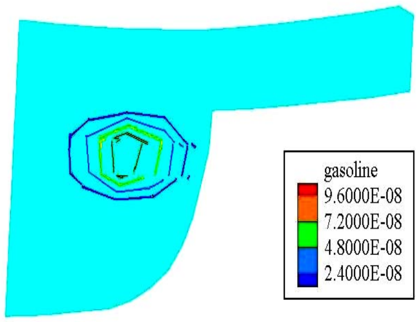


Fig. 11: Gasoline mass fraction

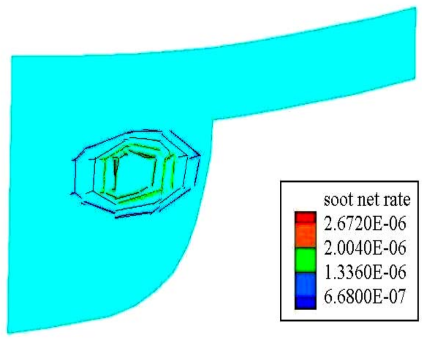


Fig. 12: Soot net rate

6. CONCLUSION

In this paper, we reviewed briefly soot model that have been proposed for diesel engine simulations. A direct injection diesel spray combustion model has been developed and implemented in a full cycle simulation of a supercharged Engine for the purpose of predicting engine performance soot emissions.

The soot modeling on a platform of a 3-dimensional CFD code requires a complex approach. The first step was carried out by the simulation of compression and expansion strokes of the investigated engine including combustion.

The results of the soot model are influenced by numerical constants, value of which should be chosen from a recommended range.

The two-step empirical soot model is easily implemented and adjusted, but the present results show that caution must be paid when considering the predicted spatial distribution.

NOMENCLATURE

ATDC	After Top Dead Center
BTDC	Before Top Dead Center
$C_n H_n$	Hydrocarbon
E_i	Activity temperature
K	Degree Kelvin (temperature)
P	Pressure
R_{pm}	Crankshaft r.p.m.
R	Universal gas constant
SOI	Start of injection
T	Temperature
t	Time
TDC	Top Dead Center

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